

Parity nonconservation in hyperfine transitions

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We use relativistic Hartree-Fock and correlation potential methods to calculate nuclear spin-dependent parity non-conserving amplitudes (dominated by the nuclear anapole moment) between hyperfine structure components of the ground state of odd isotopes of K, Rb, Cs, Ba⁺, Yb⁺, Tl, Fr, and Ra⁺. The results are to be used for interpretation of current and future measurements.

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I. INTRODUCTION

Current best atomic test of the standard model comes from the measurements [1] and interpretation [2] of the parity-nonconservation (PNC) in atomic cesium (see also review [3]). The PNC effect measured in cesium is dominated by the nuclear spin-independent contribution due to the weak nuclear charge Q_W . The value of $Q_W(^{133}\text{Cs})$ extracted from the measurements is in perfect agreement with the standard model.

Since it is hard to compete with cesium PNC in terms of the accuracy of the interpretation of the measurements, the focus of the atomic PNC studies has shifted mostly to the study of the nuclear spin-dependent PNC effects (dominated by the nuclear P-odd anapole moment) and PNC in the chain of isotopes. The anapole moments has been measured so far only for the nucleus of ^{133}Cs [1]. The information about weak nuclear forces extracted from these measurements seems to be inconsistent with the information obtained from the limit on the nuclear anapole extracted from the thallium PNC [4, 5] and some other sources (see, e.g. [3]). Therefore, it would be very important to get more anapole measurements. The experiments are in progress or planned for Yb and Dy at Berkeley [6, 7], Yb⁺ at Los Alamos [8], Ra⁺ at KVI [9, 10], Rb and Fr at TRIUMF [11, 12]. There were also proposals to measure atomic PNC in K [14], Ba⁺ [15], and Xe [16]. Most of these experiments are aimed at both, nuclear spin-dependent PNC effects and PNC in a chain of isotopes. The proposals for K [14], Rb and Fr [11, 12] specifically target the effect of the the nuclear anapole moment in atomic hyperfine transitions. The interpretation of these measurements requires atomic calculations. Note that PNC in the Zeeman transitions considered in Ref. [13] is also based on such calculations.

Nuclear spin-dependent PNC effects in hyperfine transitions were considered semiempirically in Refs. [17, 18]. *Ab initio* calculations for Fr, which included correlations, core polarization and Breit interaction were reported in Ref. [19]. Ref. [20] presents calculations of the nuclear spin-dependent PNC for a wide range of single-valence-electron atoms. The calculations are in random phase approximation (RPA) which means that core polariza-

tion is included.

In present paper we perform calculations of the nuclear spin-dependent PNC for a range of atoms of potential experimental interest. These includes K, Rb, Cs, Fr, Tl, Ba⁺, Ra⁺, and Yb⁺. We have included the core polarization (RPA) and correlation effects. The results in the RPA approximation are in perfect agreement with Ref. [20]. The inclusion of the correlations in our work increases the PNC amplitudes by 3 to 7%. The relatively small magnitude of the correlation corrections is due to cancelation of different contributions. Based on the detailed study of the error budget in Ref. [2], we expect that the accuracy of present calculations is few per cent. The agreement with Ref. [19] for Fr is not so good, and we discuss the reasons for the difference.

II. THEORY

Hamiltonian describing the nuclear spin dependent parity-nonconserving electron-nuclear interaction can be written in a form (we use atomic units: $\hbar = |e| = m_e = 1$):

$$H_{\text{SD-PNC}} = \frac{G_F}{\sqrt{2}} \frac{\kappa}{I} \boldsymbol{\alpha} \mathbf{I} \rho(\mathbf{r}), \quad (1)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$ is the Dirac matrix, \mathbf{I} is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1. The strength of the spin-dependent PNC interaction is proportional to the dimensionless constant κ which is to be found from the measurements. There are three major contributions to κ arising from (i) electromagnetic interaction of atomic electrons with nuclear *anapole moment* [21], (ii) electron-nucleus spin-dependent weak interaction [17, 22], and (iii) combined effect of the spin-independent weak interaction and the magnetic hyperfine interaction [23] (see also review [3]). In this work we do not distinguish between different contributions to κ and present the results in terms of total κ which is the sum of all possible contributions (the nuclear anapole gives the dominating contribution in heavy atoms).

The PNC amplitude of an electric dipole transition between states of the same parity $|i\rangle$ and $|f\rangle$ is equal to:

$$E1_{fi}^{PNC} = \sum_n \left[\frac{\langle f|\mathbf{d}|n\rangle\langle n|H_{PNC}|i\rangle}{E_i - E_n} + \frac{\langle f|H_{PNC}|n\rangle\langle n|\mathbf{d}_q|i\rangle}{E_f - E_n} \right], \quad (2)$$

where $\mathbf{d} = -e \sum_i \mathbf{r}_i$ is the electric dipole operator, $|a\rangle \equiv |J_a F_a M_a\rangle$ and $\mathbf{F} = \mathbf{I} + \mathbf{J}$ is the total angular momentum.

Applying the Wigner-Eckart theorem we can express the amplitudes via reduced matrix elements

$$E1_{fi}^{PNC} = (-1)^{F_f - M_f} \begin{pmatrix} F_f & 1 & F_i \\ -M_f & q & M_i \end{pmatrix} \times \langle J_f F_f || d_{PNC} || J_i F_i \rangle. \quad (3)$$

Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found e.g. in Refs. [19] and [20]. For the SD PNC amplitude we have

$$\begin{aligned} \langle J_f, F_f || d_{SD} || J_i, F_i \rangle &= \frac{G_F}{\sqrt{2}} \kappa \\ &\times \sqrt{(I+1)(2I+1)(2F_i+1)(2F_f+1)/I} \\ &\times \sum_n \left[(-1)^{J_f - J_i} \begin{Bmatrix} J_n & J_i & 1 \\ I & I & F_i \end{Bmatrix} \begin{Bmatrix} J_n & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \right. \\ &\times \frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || \boldsymbol{\alpha} \rho || J_i \rangle}{E_n - E_i} \\ &+ (-1)^{F_f - F_i} \begin{Bmatrix} J_n & J_f & 1 \\ I & I & F_f \end{Bmatrix} \begin{Bmatrix} J_n & J_i & 1 \\ F_i & F_f & I \end{Bmatrix} \\ &\left. \times \frac{\langle J_f || \boldsymbol{\alpha} \rho || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_n - E_f} \right]. \quad (4) \end{aligned}$$

This formula can be used for optical and microwave transitions. For the microwave transitions it can be further simplified as it has been done in Ref. [19].

To calculate the PNC amplitudes we use direct summation over a complete set of single-electron states constructed using the B-spline technique [24]. Correlations and core polarization effects are included by means of the correlation potential method [25]. The calculations are very similar to those of our previous work [26], therefore we omit here the details.

III. RESULTS

The results of calculations are presented in Table I. The results of present work for the PNC amplitude are presented in two different approximations, the RPA approximation, which includes core polarization but no correlations beyond it, and final results which include core polarization and Brueckner-type correlations. The results of Ref. [20], which were obtained in the RPA approximation, are also presented for comparison. For the

convenience of the comparison we present the results for the PNC amplitudes in a form which corresponds to the PNC Hamiltonian, used in [20]:

$$H_{SD-PNC} = \frac{G_F}{\sqrt{2}} \xi \boldsymbol{\alpha} \mathbf{I} \rho(\mathbf{r}). \quad (5)$$

It differs from (1) by the use of the different weak interaction constant ξ ($\xi = \kappa/I$).

The RPA results of [20] and present work are in perfect agreement with each other. The inclusion of Brueckner-type correlations increase the PNC amplitudes by 3 to 7%. It is interesting to note that the correlation correction is larger for light elements and slowly decrease for higher Z .

In Table I we also present the values of the reduced matrix elements for the magnetic dipole ($M1$) transition amplitudes between corresponding hyperfine states and the degrees of circular polarization of light P . The $M1$ amplitudes are given by

$$\begin{aligned} \langle F, J || M1 || F', J \rangle &= (-1)^{I+J+F} g(J, L) \mu_B \\ &\times \sqrt{(2F+1)(2F'+1)J(J+1)(2J+1)} \begin{Bmatrix} F & 1 & F' \\ J & I & J \end{Bmatrix}, \quad (6) \end{aligned}$$

where $g(J, L)$ is the g -factor of atomic state $J, L, S = 1/2$

$$g(J, L) = 1 + \frac{J(J+1) - L(L+1) + \frac{3}{4}}{2J(J+1)}, \quad (7)$$

J, L are atomic total and angular momentums, and $\mu_B = |e|\hbar/2mc$ is Bohr magneton. In the case of $J = 1/2, F = I \pm 1/2$ the Eq. (6) can be further reduced to

$$M1 = 2 \sqrt{\frac{I(I+1)}{I + \frac{1}{2}}} \left[1 - \frac{L(L+1)}{3} \right] \mu_B. \quad (8)$$

The degree of the circular polarization of light is given by

$$P = 2 \frac{Im(E1)}{M1}. \quad (9)$$

The results for ^{211}Fr , converted to a different definition of the weak interaction constant ($\kappa = \xi I$) consistent with Hamiltonian (1), are $0.529 \times 10^{-10} i\kappa$ [20] and $0.553 \times 10^{-10} i\kappa$ (present work). They differ by only 4.5% and this difference is due to correlations which were included in the present work but not included in Ref. [20]. On the other hand, the difference between the result of present work and the calculations by Porsev and Kozlov [19], which is $0.491 \times 10^{-10} i\kappa$, is significantly larger, being about 13%. It is important to understand the reason for this difference, since the calculations by Porsev and Kozlov are the only other calculations for Fr which included correlations beyond the RPA approximation. The experimental work for Fr is in progress at TRIUMF [11, 12] and for its future interpretation it is important to have reliable theoretical results.

TABLE I: Reduced matrix elements of the nuclear spin-dependent weak interaction for microwave transitions between ground-state hyperfine levels F_1, F_2 in atoms and ions of potential experimental interest. In this table, Z is the nuclear charge, A is the atomic number, I is the nuclear spin, the hyperfine levels have angular momentum $F = I \pm 1/2$, M_1 is magnetic dipole transition amplitude, P is the degree of circular polarization. All dimensional numbers are in atomic units. The values for M_1 amplitudes include Bohr magneton ($\mu_B = \alpha/2$ in atomic units). The PNC amplitudes and circular polarization P are proportional to the weak interaction constant ξ (5) which is omitted from the table. Numbers in square brackets represent powers of 10.

Atom	Z	A	I	F_1	F_2	RPA Ref. [20]	RPA	RPA+ Σ this work	M_1	P
K	19	39	3/2	2	1	2.222[-13]	2.222[-13]	2.378[-13]	0.0100	4.76[-11]
Rb	37	85	5/2	3	2	2.550[-12]	2.532[-12]	2.660[-12]	0.0125	4.27[-10]
Rb	37	87	3/2	2	1	1.363[-12]	1.353[-12]	1.422[-12]	0.0100	2.85[-10]
Cs	55	133	7/2	4	3	1.724[-11]	1.720[-11]	1.819[-11]	0.0145	2.51[-09]
Ba ⁺	56	135	3/2	2	1	6.169[-12]	6.186[-12]	6.385[-12]	0.0100	1.28[-09]
Yb ⁺	70	171	1/2	1	0		3.844[-12]	3.987[-12]	0.0063	1.26[-09]
Yb ⁺	70	173	5/2	3	2		2.274[-11]	2.359[-11]	0.0125	3.79[-09]
Tl	81	203	1/2	1	0	3.000[-11]	3.001[-11]	3.066[-11]	0.0021	2.92[-08]
Fr	87	211	9/2	5	4	2.379[-10]	2.362[-10]	2.487[-10]	0.0162	3.07[-08]
Fr	87	223	3/2	2	1	5.820[-11]	5.815[-11]	6.051[-11]	0.0100	1.21[-08]
Ra ⁺	88	223	3/2	2	1	5.987[-11]	5.991[-11]	6.147[-11]	0.0100	1.23[-08]

TABLE II: Contributions to the $6s - 7s$ E_{PNC} for Cs in units $10^{-11} i e a_B (-Q_W/N)$. First line is equivalent to the approximation used in present work.

Brueckner orbitals + core polarization	0.9077
Weak correlation potential	0.0038
Structural radiation	0.0029
Normalization	-0.0066
Breit correction	-0.0055
Neutron distribution	-0.0018
Radiative corrections ^a	-0.0029
Total	0.8976

^aRef. [27]

The most obvious difference between present calculations and those of Ref. [19] is inclusion of higher-order correlations in our work and some small effects in [19]. These small effects include Breit interaction, structural radiation and renormalization of wave functions. We first discuss these small corrections. The most detailed study of all important corrections to the PNC amplitude has been done for the $6s - 7s$ PNC amplitude for Cs [2, 27]. The results are summarized in Table II. The relative values of specific corrections for the hfs PNC transition in Fr might be slightly different, however, the qualitative picture should be very similar. First line in Table II corresponds to the approximation used in the present work. Note that the final result is only about 1% smaller. Furthermore, there is strong cancelation between different contributions. For example, the contributions from the weak correlation potential and the structural radiation are canceled by the renormalization of the wave functions. Different contributions to the radiative corrections are not so small (up to -0.8%). However, they have different signs and nearly cancel each other. This means

TABLE III: Reduced matrix elements of the nuclear spin-dependent PNC amplitude $\langle 7s, F = 5 || d_{\text{PNC}} || 7s, F = 4 \rangle$ for ^{211}Fr in units $\times 10^{-10} i \mathcal{Z}$. To compare these numbers with those presented in Table I one should multiply them by the nuclear spin $I = 9/2$. Contributions from the core are not included in first three columns.

	DHF	RPA	MBPT ^a	core	Total
Porsev and Kozlov [19]	0.418	0.058	0.033	-0.018	0.491
this work	0.423	0.058	0.009	0.063	0.553

^aMany-body perturbation theory for the correlation correction.

that inclusion of some of the small corrections while not including others cannot be justified and may lead to less accurate results.

We proceed to the examining the correlations. For this purpose we compare our results with those from Ref. [19] term by term as it is shown in Table III. The first column shows the PNC amplitude in the Dirac-Hartree-Fock approximation without any correlations. There is a small, about 1% difference in the results. Some of this difference might be attributed to the Breit interaction which is included in [19] and not included in our work. There might be also some difference due to different treatment of the nucleus. We use smooth Fermi distribution of the nuclear electric charge and anapole moment, while a step-like function is used in [19].

The RPA correction is the same in both works (see Table III). The difference in correlation correction is significant which is not surprising due to very different treatment of the correlations in two works. We include the dominating Brueckner-type correlations with the use of the all-order correlation potential Σ [26]. The correlations are included in Ref. [19] in the second-order only, including the structure radiation and the renormalization

of the wave functions. These latter corrections are small (see discussion above) and cannot explain the difference in the results.

To test whether the difference is due to the higher-order correlations we performed calculations in which all higher-order correlations were removed. The correlation potential Σ was calculated in the second order and the core polarization corrections were not included. The result, $0.021 \times 10^{-10} i\hbar$, is in a reasonable agreement with [19]. In the end, the difference in the results due to different treatment of the correlations is about 5%. This difference is most likely due to the higher-order correlations included in the present work.

The largest difference comes from the contribution of the core states. This contribution is small and negative in Ref. [19]. In our calculations it is not so small and it is positive (see Table III). The value of this correction in [19] suggests that RPA corrections were probably not included. Our value for the core contributions without RPA corrections is $+0.015 \times 10^{-10} i\hbar$. However, there is no clear explanation for the different sign. Note, that we do not distinguish between core and excited states in the summation over complete set of states in (4). This leaves no room for a sign error. On the other hand, to the best of our knowledge, the contribution of the core states was calculated separately in Ref. [19].

There is a simple test to check the sign of the core contribution. The summation over core states in (4) is dominated by the $6p_{1/2}$ state, while summation above core is dominated by the $7p_{1/2}$ state. The angular coefficients in (4) are the same for core and higher states. One needs only to compare the energy denominators and the matrix elements of weak and electric dipole interactions. The energy denominators $E_{7s} - E_{6p_{1/2}}$ and $E_{7s} - E_{7p_{1/2}}$ are of the opposite sign. To compare the signs of matrix elements we need to fix the phase of the wave functions. It is convenient to have $f(r) > 0$ at $r \rightarrow 0$, where $f(r)$

is the upper component of the Dirac spinor. Then, the $\langle 7s || H_{\text{PNC}} || 6p_{1/2} \rangle$ and $\langle 7s || H_{\text{PNC}} || 7p_{1/2} \rangle$ matrix elements have the same sign since the values of these matrix elements comes from short distances where the $6p_{1/2}$ and $7p_{1/2}$ functions are proportional to each other [28]. In contrast, the signs of the $\langle 7s || d || 6p_{1/2} \rangle$ and $\langle 7s || d || 7p_{1/2} \rangle$ matrix elements are different since their value comes from large distances where the $6p_{1/2}$ and $7p_{1/2}$ functions have different sign. This statement can be checked using the simplest possible approximation, e.g. the DHF approximation. The many body corrections are not large enough to change the sign of the electric dipole matrix elements.

In our previous work [28], we used the results of Ref. [19] and the ratio of the matrix elements of spin-dependent PNC interaction and electron electric dipole moment (EDM) to extract the value of the EDM enhancement factor for Fr from the spin-dependent PNC calculations of [19]. The result, $d(\text{Fr}) = 854d_e$, was in reasonably good agreement with the many-body calculations of Ref. [29], $d(\text{Fr}) = 910(46)d_e$. We can use the result of present work instead of [19] for the same purpose. First, we need to remove the contribution of the $p_{3/2}$ states to use the proportionality of the matrix elements. This reduces the PNC amplitude for ^{211}Fr to $0.523 \times 10^{-10} \hbar$. The resulting EDM enhancement factor $d(\text{Fr}) = 911$ is even in better agreement with the result 910(46) of Ref. [29]. This is a good consistency test of the calculations.

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- [1] C. S. Wood, S. C. Bennett, D. Cho, B. P. Masterson, J. L. Roberst, C. E. Tanner, C. E. Wieman, *Science* **275**, 1759 (1997).
 - [2] V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, *Phys. Rev. D* **66**, 076013 (2002); S. G. Porsev, K. Beloy, and A. Derevianko, *Phys. Rev. Lett.* **102**, 181601 (2009); S. G. Porsev, K. Beloy, and A. Derevianko, *Phys. Rev. D* **82**, 036008 (2010).
 - [3] J. S. M. Ginges and V. V. Flambaum, *Phys. Rep.* **397**, 63 (2004).
 - [4] P. A. Vetter, D. M. Meekhof, P. K. Majumder, S. K. Lamoreaux, and E. N. Fortson, *Phys. Ref. Lett.* **74**, 2658 (1995).
 - [5] M. G. Kozlov, *Pis'ma Zh. Eksp. Teor. Fiz.* **75**, 651 (2002) [*Sov. Phys. JETP Lett.* **75**, 534 (2002)].
 - [6] K. Tsigutkin, D. Dounas-Frazer, A. Family, J. E. Stalnaker, V. V. Yashchuk, and D. Budker, *Phys. Rev. Lett.* **103**, 071601 (2009); *Phys. Rev. A* **81**, 032114 (2010).
 - [7] A. T. Nguyen, D. Budker, D. DeMille, and M. Zolotarev, *Phys. Rev. A* **56**, 3453 (1997).
 - [8] J. Torgerson, private communication (2010).
 - [9] L. W. Wansbeek *et al*, *Phys. Rev. A* **78**, 050501(R) (2008).
 - [10] O. O. Versolato *et al*, *Phys. Rev. A* **82**, 010501(R) (2010).
 - [11] D. Sheng, L. A. Orozco, and E. Gomez, *J. Phys. B* **43**, 074004 (2010).
 - [12] E. Gomez, L. A. Orozco, and G. D. Sprouse, *Rep. Prog. Phys.* **69**, 79 (2006).
 - [13] E. J. Angstmann, T. H. Dinh, and V. V. Flambaum, *Phys. Rev. A* **72**, 052108 (2005).
 - [14] V. F. Ezhov, M. G. Kozlov, G. B. Krygin GB, *et al*, *Tech. Phys. Lett.* **30**, 917 (2004).
 - [15] N. Fortson, *Phys. Rev. Lett.* **70**, 2383 (1993).
 - [16] D. Budker and T. P. Rakitzis, private communication (2011).
 - [17] V. N. Novikov and I. B. Khriplovich, *Pis'ma Zh. Eksp. Teor. Fiz.* **22**, 162 (1975) [*JETP Lett.* **22**, 74 (1975)].
 - [18] V. G. Gorshkov, V. F. Ezhov, M. G. Kozlov, and A. I.

- Mikhailov, *Yad. Fiz.* **48**, 1363 (1988) [*Sov. J. Nucl. Phys.* **48**, 867 (1988)].
- [19] S. G. Porsev and M. G. Kozlov, *Phys. Rev. A* **64**, 064101 (2001).
 - [20] W. R. Johnson, M. S. Safronova, and U. I. Safronova, *Phys. Rev. A* **67**, 062106 (2003).
 - [21] V. V. Flambaum, I. B. Khriplovich, *ZhETP* **79**, 1656 (1980) (*Soviet Phys. JETP* **52**, 835 (1980)). V.V. Flambaum, I.B. Khriplovich, O.P. Sushkov. *Phys. Lett. B.* **146**, 367, 1984.
 - [22] V. N. Novikov, O. P. Sushkov, V. V. Flambaum, I. B. Khriplovich, *ZhETP* **73**, 802 (1977) (*Soviet Phys. JETP* **46**, 420 (1977)).
 - [23] V. V. Flambaum, I. B. Khriplovich, *ZhETP* **89**, 1505 (1985) (*Soviet Phys. JETP* **62**, 872 (1985)).
 - [24] W. R. Johnson, and J. Sapirstein, *Phys. Rev. Lett.* **57**, 1126 (1986).
 - [25] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, O. P. Sushkov, *J. Phys. B* **20**, 1399 (1987).
 - [26] V. A. Dzuba and V. V. Flambaum, *Phys. Rev. A* **83**, 052513 (2011).
 - [27] V. V. Flambaum and J. S. M. Ginges, *Phys. Rev. A* **72**, 052115 (2005).
 - [28] V. A. Dzuba, V. V. Flambaum, and C. Harabati, *Phys. Rev. A* **84**, 052108 (2011).
 - [29] T. M. R. Byrnes, V. A. Dzuba, V. V. Flambaum, and D. W. Murray, *Phys. Rev. A*, **59**, 3082 (1999).